Pseudogap in the one-electron spectral functions of the attractive Hubbard model

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We calculate the one-electron Green's function of the 2D attractive Hubbard model by coupling the electrons to pair fluctuations. The latter are approximated by homogeneous amplitude fluctuations and phase correlations corresponding to the XY-model. The electronic density of states shows a pseudogap at temperatures well above the transition temperature T_C. For a quasi-3D system, a superconducting gap emerges out of the pseudogap below T_C.

The 2D attractive Hubbard model is treated by a Stratonovich-Hubbard transformation (SHT), decoupling the interaction term by a complex pairing field Δ. The one-electron Green's function is then approximately given by [1]:

$$G\left(\vec{k}, z_\nu\right)^{-1} = z_\nu - \epsilon_{\vec{k}} + \mu - \sigma\left(\vec{k}, z_\nu\right) - \frac{\langle\Delta\rangle^2}{z_\nu + \epsilon_{\vec{k}} - \mu + \sigma\left(\vec{k}, -z_\nu\right)}. \tag{1}$$

The expression for the self-energy

$$\sigma\left(\vec{k}, z_\nu\right) = -\sum_{\vec{q}} \sum_{z_\alpha} \left\langle |\Delta\left(\vec{q}, z_\alpha\right)|^2 \right\rangle G\left(\vec{k} - \vec{q}, z_\nu - z_\alpha\right), \tag{2}$$

involves the dynamic correlation function of the pairing field, which is related to the one-electron propagator through the SHT. However, rather than aiming at a self-consistent solution, we adopt a simple form for the pairing correlations and study their influence on the one-electron properties. Introducing amplitude and phase, $\Delta\left(\vec{r}, t\right) = |\Delta\left(\vec{r}, t\right)| e^{i\theta(\vec{r},t)}$, we make the following assumptions :

(i) Below the temperature T^*, the amplitude fluctuations (assumed to be space- and time-independent) are approximated by a BCS-form, $\langle|\Delta|^2\rangle = \Phi_0\left(1 - \frac{T}{T^*}\right)$, with a prefactor Φ_0 that allows to vary their strength. The average $\langle\Delta\rangle$ is zero. The strong anisotropy of underdoped compounds shows that the coupling between the planes is weak. Thus, we model the phase fluctuations as in a 2D-XY system. Above the critical temperature T_C, we approximate it by a dispersionless relaxation [2,3] :

$$\left\langle e^{i\left(\theta(\vec{r},t) - \theta(\vec{0},t)\right)} \right\rangle = e^{-\gamma t} \left(\frac{r_0}{r_0 + r}\right)^{\eta(T)} e^{-\frac{r}{\xi_+(T)}}, \tag{3}$$

with a Berezinskii-Kosterlitz-Thouless correlation length $\xi_+(T) = \xi_0 e^{\frac{b}{\sqrt{T - T_C}}}$ and a relaxation frequency γ.

(ii) Below the critical temperature T_C we keep, for simplicity, the same form (3) for the phase correlations, but with $\xi^{-1} = 0$, corresponding to an algebraic decay of correlations. Taking into account a non-zero coupling between the planes (in the third dimension), we introduce a non-zero value for the average of Δ, $\langle\Delta\rangle^2 = \lambda\langle|\Delta|^2\rangle$, with a variable parameter $\lambda \leq 1$.

We then evaluate $\sigma\left(\vec{k}, z_\nu\right)$ to lowest order by using the non-interacting Green's function and the isotropic spectrum $\epsilon\left(\vec{k}\right) = \frac{k^2}{2m} - \mu$ in expression (2). The wave-number integration is limited to an effective spherical Brillouin zone. The various parameters are chosen to describe high-T_C materials in the strongly underdoped regime, where the pseudogap is most pronounced : the (fixed) chemical potential $\mu = \frac{k_F^2}{2m}$ is taken to correspond to about 0.1 charge

carrier per site and $k_B T^* = \mu$, $T_C = \frac{T^*}{6}$.

On the figures, we show the electronic density of states $N(E)$ and some spectral functions for $\Phi_0 = 0.76$ and $\gamma = 0.5\mu$. The following observations can be made :

(i) Above T_C, a pseudogap opens around μ. Its effective width is almost T-independent, in spite of the T-dependence of $\langle |\Delta|^2 \rangle$ in the self-energy. Near T^*, it is roughly V-shaped. By approaching T_C, it becomes more U-shaped (for our model, pairing is s-like) and $N(\mu)$ becomes then practically zero; the pseudogap is delimited by two rather pronounced maxima, although $\langle \Delta \rangle$ is still zero.

(ii) Below T_C, the presence of $\langle \Delta \rangle \neq 0$ produces two new peaks: a true "superconducting gap" emerges out of the pseudogap. Its width is given by the geometrical superposition of average and fluctuating part of Δ. The fluctuations of the latter remain visible in the form of secondary shoulders inside the superconducting gap which approach each other about in the same proportion as the main peaks move away from each other.

(iii) Our value for γ is relatively large. For a smaller γ, and in particular in the case of critical slowing down of phase fluctuations ($\gamma\left(T_C^+\right) = 0$) [2] the two shoulders would become secondary peaks inside the superconducting gap.

(iv) Near T_C, the spectral functions are doubly peaked in some wave-vector domain around k_F and the width of the pseudogap is given by the separation between these two peaks, which is essentially determined by $\langle |\Delta|^2 \rangle$. At higher temperatures, the spectral functions have only one peak, but their width is enhanced over essentially the same k-domain. Due to this fact, the pseudogap is filling up gradually, when T^* is approached (from below), without changing very much its width.

Summarizing, we have evaluated the electronic density of states of the attractive Hubbard model, taking into account the coupling of the charge carriers to the fluctuating pairing field. The appearance of a pseudogap with a T-independent width and the emergence of a superconducting gap below T_C is in agreement with experimental findings (see for example [4]). In a future publication, we shall present more detailed results and also compare the latter with the ones that have been recently proposed within similar approaches [5].

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FIGURE CAPTIONS

Figure 1 : One-electron density of states $N(E)$ above T_C, for $T = 2T_C$ (dot-dashed line), $T = 1.5T_C$ (dotted line), $T = 1.2T_C$ (dashed line) and $T = 1.01T_C$ (full line).

Figure 2 : $N(E)$ below T_C for $\lambda = 0.7$ (full line) and - for comparison - above T_C ($T = 1.01T_C$, dashed line).

Figure 3 : One-electron spectral functions for $k = 0.5k_F$ (dashed line), $k = 0.7k_F$ (dotted line), $k = k_F$ (full line), $k = 1.2k_F$ (dash-dotted line), $k = 1.5k_F$ (heavy full line), for $T = 1.01T_C$ and (inset) $T = 1.5T_C$.

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